

**PACKAGE ID** - 000130DVX1100 DESUL MODEL-FLUBATCH

**KWIC TITLE** - Desulfurization Model for Batch Fluidized-Bed

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**LIMITATION CODE** - UNL

**AUDIENCE CODE** - UNL

**COMPLETION DATE** - 03/01/1988

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**DESCRIPTION** - Models were developed to complement the DOE-METC effort to develop a high-temperature process for the desulfurization of coal-derived gases. Computer models capable of describing both the sulfidation and regeneration cycles in batch fluidized-bed reactors have been written and tested. Isothermal conditions have been assumed during the sulfidation phase but the highly exothermic nature of the regeneration reactions made it necessary to consider nonisothermal regeneration.

**PACKAGE CONTENTS** - Media Directory; Software Abstract; Media Includes Source Code, Executable Module, Object Module;

**SOURCE CODE INCLUDED?** - Yes

**MEDIA QUANTITY** - 1 5.25 Diskette

**METHOD OF SOLUTION** - All models are based upon the simultaneous solution of the differential equations describing the component material balances and, where necessary, energy balances. The models are heterogeneous in that the solid and fluid phases are considered separately. Concentration and/or temperature gradients between solid and fluid phases are described in terms of mass and heat transfer coefficients. Plug flow of the gas phase is assumed. The solids are assumed to be perfectly mixed in the fluidized-bed model. The overall description of the fluidized-bed is based upon the Kunii-Levenspiel three-phase bubble model. Parameters in this model such as interphase mass transfer coefficients are developed from correlations taken from the literature. Single particles within the fluidized-bed are assumed to react homogeneously. While

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**METHOD OF SOLUTION - (CONT)** no independent studies to verify this assumption have been carried out, the model is justified on the basis of the small particle sizes used in fluidized-beds.

**COMPUTER** - DEC VAX11

**OPERATING SYSTEMS** - VMS

**PROGRAMMING LANGUAGES** - FORTRAN IV

**SOFTWARE LIMITATIONS** - None

**SOURCE CODE AVAILABLE (Y/N)** - Y

**UNIQUE FEATURES** - Only known models for hot gas desulfurization/regeneration processes for batch fluidized-bed applications.

**RELATED SOFTWARE** - This is the original software.

**OTHER PROG/OPER SYS INFO** - File naming convention used is (filename).DOC. No proprietary or any special software is required.

**HARDWARE REQS** - Standard features

**TIME REQUIREMENTS** - Less than 5 minutes

**REFERENCES** - Final report on the work performed under Contract No.: DE-AC21-86MC23089, Dynamic Simulation Models for High-Temperature Desulfurization Processes, March 1988, by Louisiana State University, DOE/MC/23089-2601, (DE88010263).

**ABSTRACT STATUS** - Submitted 11/26/91

**SUBJECT CLASS CODE** - R

**KEYWORDS** -

D CODES  
DESULFURIZATION  
COAL GAS  
FLUIDIZED BED REACTORS  
ISOTHERMAL PROCESSES  
MATHEMATICAL MODELS  
COMPUTERIZED SIMULATION  
COMPUTER PROGRAM DOCUMENTATION

**EDB SUBJECT CATEGORIES** -  
990200 010402

**SPONSOR** - DOE/FE

**PACKAGE TYPE** - SCREENED